

WHAT IS CLAIMED IS:

1 1. A spectral processing method for compensating a plurality of
2 sequential spectra and profiles derived therefrom for effects of drift comprising:
3 transforming a plurality of sequential spectra obtained from a spectrometer to
4 provide an array of drift-compensated row vectors, wherein the array of drift-
5 compensated row vectors constitutes a drift-compensated array;
6 performing a principal-factor determination on the drift-compensated array to
7 provide a set of drift-compensated principal factors; and
8 generating drift-compensated scaled target-factor profiles from a profile
9 trajectory of the drift-compensated row vectors lying within a space of drift-
10 compensated principal factors.

1 2. The spectral processing method of claim 1 further comprising
2 generating drift-compensated compositional profiles from the drift-compensated
3 scaled target-factor profiles.

1 3. The spectral processing method of claim 1, wherein the transforming
2 the plurality of sequential spectra further comprises:
3 inputting a plurality of sequential spectra from a spectrometer into a computer
4 system;
5 ordering the spectra in a primal array of row vectors, wherein each sequential
6 spectrum constitutes a successive row vector of the primal array; and
7 removing phase factors due to drift using a dephasing procedure that
8 transforms the primal array into a drift-compensated array.

1 4. The spectral processing method of claim 3 wherein the dephasing
2 procedure for transforming the primal array into the drift-compensated array further
3 comprises applying a Fourier transform to the spectra in the primal array of row
4 vectors forming an array of Fourier-transformed row vectors, multiplying each
5 Fourier-transformed row vector by a complex conjugate of each Fourier-transformed
6 row vector to form a squared moduli vector thereby removing phase factors due to
7 drift, taking the square root of each element of the squared moduli vector to create a
8 corresponding moduli vector, and forming a drift-compensated array of moduli
9 vectors by successively sequencing the moduli vectors as successive drift-
10 compensated row vectors in a drift-compensated array, wherein the moduli vectors
11 constitute moduli of Fourier-transformed spectra.

1 5. The spectral processing method of claim 4 further comprising
2 outputting the drift-compensated row vectors of the drift-compensated array as a
3 sequential series of moduli of Fourier-transformed spectra.

1 6. The spectral processing method of claim 3 wherein the dephasing
2 procedure for transforming the primal array into the drift-compensated array further
3 comprises applying a fitting procedure to each spectrum in the primal array using
4 selected reference spectra, calculating through the fitting procedure a corresponding
5 reference weighting factor for each reference spectrum corresponding to each
6 spectrum in the primal array, removing the phase factor due to drift from each
7 spectrum in the primal array by synthesizing a corresponding drift-compensated
8 spectrum given by the sum of each selected reference spectrum multiplied by the

9 corresponding reference weighting factor, and forming a drift-compensated array by
10 successively sequencing the drift-compensated spectra as successive drift-
11 compensated row vectors in the drift-compensated array.

1 7. The spectral processing method of claim 6 further comprising
2 outputting analytical results selected from the group consisting of the selected
3 reference spectra used in the fitting procedure, the drift-compensated row vectors of
4 the drift-compensated array as a sequential series of drift-compensated spectra,
5 reference weighting factors for each reference spectrum corresponding to each
6 spectrum in the primal array as a set of drift-compensated reference-spectrum
7 profiles, and phase factors due to drift for each reference spectrum corresponding to
8 each spectrum in the primal array as a set of phase-factor profiles.

1 8. The spectral processing method of claim 1 wherein the performing the
2 principal-factor determination comprises performing a factor analysis.

1 9. The spectral processing method of claim 8, wherein the performing the
2 factor analysis further comprises:

3 forming a covariance array from the drift-compensated array;
4 applying an eigenanalysis to the covariance array to define a complete set of
5 eigenvectors and eigenvalues; and
6 defining a set of drift-compensated principal factors by selecting a subset of
7 eigenvectors from the complete set of eigenvectors.

1 10. The spectral processing method of claim 9, wherein the defining the

2 set of drift-compensated principal factors further comprises selecting the drift-
3 compensated principal factors as a first few eigenvectors corresponding to
4 eigenvalues above a certain limiting value.

1 11. The spectral processing method of claim 1 wherein the performing the
2 principal-factor determination comprises performing a linear-least-squares analysis.

1 12. The spectral processing method of claim 11, wherein the performing a
2 linear-least-squares analysis further comprises:

3 selecting a set of initial factors from the set of drift-compensated row vectors
4 of the drift-compensated array;

5 performing a linear-least-squares decomposition with the set of initial factors
6 on the drift-compensated row vectors in the drift-compensated array to provide a set
7 of residue factors; and

8 performing a Gram-Schmidt orthonormalization on the combined set of initial
9 factors and residue factors to provide drift-compensated principal factors.

1 13. The spectral processing method of claim 1, wherein the generating
2 drift-compensated scaled target-factor profiles further comprises:

3 constructing a set of drift-compensated target factors on a space of the drift-
4 compensated principal factors;

5 applying the set of drift-compensated target factors to a profile trajectory lying
6 within a space of drift-compensated principal factors to obtain a sequential set of
7 target-factor weighting factors corresponding to the drift-compensated target factors

8 for the profile trajectory; and
9 outputting analytical results selected from the group consisting of a set of
10 drift-compensated scaled target-factor profiles derived from the set of target-factor
11 weighting factors, and the set of drift-compensated target factors.

12

1 14. The spectral processing method of claim 13, wherein the constructing
2 the set of drift-compensated target factors further comprises:

3 generating a profile trajectory on a 3-dimensional projection of a 4-
4 dimensional space of a set of first-four, drift-compensated principal factors along
5 with a reference tetrahedron the vertices of which represent each of the first-four,
6 drift-compensated principal factors;

7 enclosing the profile trajectory within an enclosing tetrahedron with vertices
8 centered on end-points and in proximity to turning points of the profile trajectory, and
9 with faces lying essentially tangent to portions of the profile trajectory; and

10 calculating the drift-compensated target factors from the normed coordinates
11 of the vertices of the enclosing tetrahedron in terms of the drift-compensated
12 principal factors.

1 15. The spectral processing method of claim 14, wherein the generating
2 the profile trajectory further comprises:

3 calculating 4-space coordinates of a profile trajectory of drift-compensated
4 target-factor profiles on a 4-dimensional space to produce four coordinates for each
5 point in the profile trajectory, one coordinate for each of the first-four, drift-
6 compensated principal factors;

7 reducing the dimensionality of the coordinates of the profile trajectory by
8 dividing each coordinate by a sum of all four 4-space coordinates to produce normed
9 coordinates for the profile trajectory; and,
10 plotting the normed coordinates for the profile trajectory in a 3-dimensional
11 space the coordinate axes of which are edges of a reference tetrahedron, the
12 vertices of which correspond to unit values for each of the first-four, drift-
13 compensated principal factors in a manner analogous to plotting of coordinates on a
14 quaternary phase diagram.

16. The spectral processing method of claim 13, wherein generating drift-
compensated compositional profiles comprises:
defining a set of drift-compensated scaled target-factor profile values as the
set of scaled target-factor weighting factors;
dividing each drift-compensated scaled target-factor profile value by a profile
sensitivity factor for each constituent corresponding to the target factor to provide a
sensitivity-scaled target-factor profile value;
normalizing the sensitivity-scaled target-factor profile value by dividing each
sensitivity-scaled target-factor profile value for a given cycle number by the sum of
all the sensitivity-scaled target-factor profile values for the given cycle number to
provide drift-compensated compositional profile values at the given cycle number;
and
outputting the drift-compensated compositional profile values as a set of drift-
compensated compositional profiles.

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1 17. A waveform processing method for compensating a plurality of
2 sequential waveforms and profiles derived therefrom for effects of drift comprising:
3 transforming a plurality of sequential waveforms obtained from a waveform-
4 source device to provide an array of drift-compensated row vectors, wherein the
5 array of drift-compensated row vectors constitutes a drift-compensated array;
6 performing a principal-factor determination on the drift-compensated array to
7 provide a set of drift-compensated principal factors; and
8 generating drift-compensated scaled target-factor profiles from a profile
9 trajectory of the drift-compensated row vectors lying within a space of drift-
10 compensated principal factors .

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1 18. The waveform processing method of claim 17, wherein the
2 transforming the plurality of sequential waveforms further comprises:
3 inputting a plurality of sequential waveforms from a waveform-source device
4 into a computer system;
5 ordering the waveforms in a primal array of row vectors, wherein each
6 sequential waveform constitutes a successive row vector of the primal array; and
7 removing phase factors due to drift using a dephasing procedure that
8 transforms the primal array into a drift-compensated array.

9

1 19. The waveform processing method of claim 18 wherein the dephasing
2 procedure for transforming the primal array into the drift-compensated array further
3 comprises applying a Fourier transform to the waveforms in the primal array of row

4 vectors forming an array of Fourier-transformed row vectors, multiplying each
5 Fourier-transformed row vector by a complex conjugate of each Fourier-transformed
6 row vector to form a squared moduli vector thereby removing phase factors due to
7 drift, taking the square root of each element of the squared moduli vector to create a
8 corresponding moduli vector, and forming a drift-compensated array of moduli
9 vectors by successively sequencing the moduli vectors as successive drift-
10 compensated row vectors in a drift-compensated array, wherein the moduli vectors
11 constitute moduli of Fourier-transformed waveforms.

1 20. The waveform processing method of claim 19 further comprising
2 outputting the drift-compensated row vectors of the drift-compensated array as a
3 sequential series of moduli of Fourier-transformed waveforms.

1 21. The waveform processing method of claim 18, wherein the dephasing
2 procedure for transforming the primal array into the drift-compensated array further
3 comprises applying a fitting procedure to each sequential waveform in the primal
4 array using selected reference waveforms, calculating through the fitting procedure a
5 corresponding reference weighting factor for each reference waveform
6 corresponding to each waveform in the primal array, removing the phase factor due
7 to drift from each waveform in the primal array by synthesizing a corresponding drift-
8 compensated waveform given by the sum of each selected reference waveform
9 multiplied by the corresponding reference weighting factor, and forming a drift-
10 compensated array by successively sequencing the drift-compensated waveforms
11 as successive drift-compensated row vectors in the drift-compensated array.

1 22. The waveform processing method of claim 21 further comprising
2 outputting analytical results selected from the group consisting of the selected
3 reference waveforms used in the fitting procedure, the drift-compensated row
4 vectors of the drift-compensated array as a sequential series of drift-compensated
5 waveforms, reference weighting factors for each reference waveform corresponding
6 to each waveform in the primal array as a set of drift-compensated reference-
7 waveform profiles, and phase factors due to drift for each reference waveform
8 corresponding to each waveform in the primal array as a set of phase-factor profiles.

1 23. The waveform processing method of claim 17 wherein the performing
2 the principal-factor determination comprises performing a factor analysis.

1 24. The waveform processing method of claim 23, wherein the performing
2 the factor analysis further comprises:
3 forming a covariance array from the drift-compensated array;
4 applying an eigenanalysis to the covariance array to define a complete set of
5 eigenvectors and eigenvalues; and
6 defining a set of drift-compensated principal factors by selecting a subset of
7 eigenvectors from the complete set of eigenvectors.

1 25. The waveform processing method of claim 24, wherein the defining the
2 set of drift-compensated principal factors further comprises selecting the drift-
3 compensated principal factors as a first few eigenvectors corresponding to
4 eigenvalues above a certain limiting value.

1 26. The waveform processing method of claim 17 wherein the performing
2 the principal-factor determination comprises performing a linear-least-squares
3 analysis.

1 27. The waveform processing method of claim 26, wherein the performing
2 a linear-least-squares analysis further comprises:
3 selecting a set of initial factors from the set of drift-compensated row vectors
4 of the drift-compensated array;
5 performing a linear-least-squares decomposition with the set of initial factors
6 on the drift-compensated row vectors in the drift-compensated array to provide a set
7 of residue factors; and
8 performing a Gram-Schmidt orthonormalization on the combined set of initial
9 factors and residue factors to provide drift-compensated principal factors.

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1 28. The waveform processing method of claim 17, wherein the generating
2 drift-compensated scaled target-factor profiles further comprises:
3 constructing a set of drift-compensated target factors on a space of the drift-
4 compensated principal factors;
5 applying the set of drift-compensated target factors to a profile trajectory lying
6 within a space of drift-compensated principal factors to obtain a sequential set of
7 target-factor weighting factors corresponding to the drift-compensated target factors
8 for the profile trajectory; and
9 outputting analytical results selected from the group consisting of a set of
10 drift-compensated scaled target-factor profiles derived from the set of target-factor

11 weighting factors, and the set of drift-compensated target factors.

12

1 29. The waveform processing method of claim 28, wherein the
2 constructing the set of drift-compensated target factors further comprises:
3 generating a profile trajectory on a 3-dimensional projection of a 4-
4 dimensional space of a set of first-four, drift-compensated principal factors along
5 with a reference tetrahedron the vertices of which represent each of the first-four,
6 drift-compensated principal factors;

7 enclosing the profile trajectory within an enclosing tetrahedron with vertices
8 centered on end-points and in proximity to turning points of the profile trajectory, and
9 with faces lying essentially tangent to portions of the profile trajectory; and
10 calculating the drift-compensated target factors from the normed coordinates
11 of the vertices of the enclosing tetrahedron in terms of the drift-compensated
12 principal factors.

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1 30. The waveform processing method of claim 29, wherein the generating
2 the profile trajectory further comprises:
3 calculating 4-space coordinates of a profile trajectory of drift-compensated
4 target-factor profiles on a 4-dimensional space to produce four coordinates for each
5 point in the profile trajectory, one coordinate for each of the first-four, drift-
6 compensated principal factors;
7 reducing the dimensionality of the coordinates of the profile trajectory by
8 dividing each coordinate by a sum of all four 4-space coordinates to produce normed

9 coordinates for the profile trajectory; and,
10 plotting the normed coordinates for the profile trajectory in a 3-dimensional
11 space the coordinate axes of which are edges of a reference tetrahedron, the
12 vertices of which correspond to unit values for each of the first-four, drift-
13 compensated principal factors in a manner analogous to plotting of coordinates on a
14 quaternary phase diagram.

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1 31. An apparatus for compensating a plurality of sequential spectra and
2 profiles derived therefrom for effects of drift comprising a spectroscopic analysis
3 system, wherein the spectroscopic analysis system comprises:
4 a spectrometer; and
5 a computer system, coupled to the spectrometer, for analyzing spectra input
6 from the spectrometer, the computer system further comprising a spectral processor
7 for compensating a plurality of sequential spectra and profiles derived therefrom for
8 effects of drift.

1 32. The apparatus of claim 31, wherein the spectrometer comprises an
2 electron spectrometer.

1 33. The apparatus of claim 32, wherein the electron spectrometer
2 comprises an Auger spectrometer.

1 34. The apparatus of claim 32, wherein the electron spectrometer
2 comprises an x-ray photoelectron spectrometer.

1 35. The apparatus of claim 32, wherein the electron spectrometer
2 comprises an electron energy loss spectrometer.

1 36. The apparatus of claim 31, wherein the spectral processor further
2 comprises:

3 a spectral transformer operating on a plurality of sequential spectra obtained
4 from the spectrometer to provide an array of drift-compensated row vectors, wherein
5 the array of drift-compensated row vectors constitutes a drift-compensated array;
6 a principal-factor determinator operating on the drift-compensated array to
7 provide a set of drift-compensated principal factors; and
8 a profile generator operating on a profile trajectory of the drift-compensated
9 row vectors lying within a space of drift-compensated principal factors to provide a
10 set of drift-compensated scaled target-factor profiles.

1 37. The apparatus of claim 36, wherein the profile generator operating on
2 the set drift-compensated scaled target-factor profiles generates a set of drift-
3 compensated compositional profiles.

1 38. The apparatus of claim 36, wherein the spectral transformer accepts
2 as input the plurality of sequential spectra obtained from the spectrometer into the
3 computer system, orders the spectra in a primal array, wherein each sequential
4 spectrum constitutes a successive row vector of the primal array, and removes
5 phase factors due to drift using a dephasor that transforms the primal array into a
6 drift-compensated array.

1 39. The apparatus of claim 38, wherein the dephasor that transforms the
2 primal array into the drift-compensated array applies a Fourier transform to the
3 spectra in the primal array of row vectors to form an array of Fourier-transformed
4 row vectors, multiplies each Fourier-transformed row vector by a complex conjugate
5 of each Fourier-transformed row vector to form a squared moduli vector thereby
6 removing phase factors due to drift, takes the square root of each element of the
7 squared moduli vector to create a corresponding moduli vector, and forms a drift-
8 compensated array of moduli vectors by successively sequencing the moduli vectors
9 as successive drift-compensated row vectors in a drift-compensated array, wherein
10 the moduli vectors constitute moduli of Fourier-transformed spectra.

1 40. The apparatus of claim 39 wherein the spectral transformer outputs to
2 an output device the drift-compensated row vectors of the drift-compensated array
3 as a sequential series of moduli of Fourier-transformed spectra.

1 41. The apparatus of claim 38, wherein the dephasor that transforms the
2 primal array into the drift-compensated array fits each spectrum in the primal array
3 using selected reference spectra, calculates a corresponding reference weighting
4 factor for each reference spectrum corresponding to each spectrum in the primal
5 array, synthesizes a corresponding drift-compensated spectrum given by the sum of
6 each selected reference spectrum multiplied by the corresponding reference
7 weighting factor thereby removing phase factors due to drift, and forms a drift-
8 compensated array by successively sequencing the drift-compensated spectra as
9 successive drift-compensated row vectors in the drift-compensated array.

1 42. The apparatus of claim 41 wherein the spectral transformer outputs to
2 an output device analytical results selected from the group consisting of the selected
3 reference spectra used in the fitting procedure, the drift-compensated row vectors of
4 the drift-compensated array as a sequential series of drift-compensated spectra,
5 reference weighting factors for each reference spectrum corresponding to each
6 spectrum in the primal array as a set of drift-compensated reference-spectrum
7 profiles, and phase factors due to drift for each reference spectrum corresponding to
8 each spectrum in the primal array as a set of phase-factor profiles.

1 43. The apparatus of claim 36 wherein the principal-factor determinator
2 comprises a factor analyzer.

1 44. The apparatus of claim 43, wherein the factor analyzer forms a
2 covariance array from the drift-compensated array, applies an eigenanalysis to the
3 covariance array to define a complete set of eigenvectors and eigenvalues, and
4 defines a set of drift-compensated principal factors as a subset of eigenvectors
5 determined by a selector operating on the complete set of eigenvectors.

1 45. The apparatus of claim 44, wherein the selector operates on the
2 complete set of eigenvectors to define the set of drift-compensated principal factors
3 as a first few eigenvectors corresponding to eigenvalues above a certain limiting
4 value.

1 46. The apparatus of claim 36 wherein the principal-factor determinator
2 comprises a linear-least-squares analyzer.

1 47. The apparatus of claim 46, wherein the linear-least-squares analyzer
2 selects a set of initial factors from the set of drift-compensated row vectors of the
3 drift-compensated array, performs a linear-least-squares decomposition with the set
4 of initial factors on the drift-compensated row vectors in the drift-compensated array
5 to provide a set of residue factors, and performs a Gram-Schmidt orthonormalization
6 on the combined set of initial factors and residue factors to provide drift-
7 compensated principal factors.

1 48. The apparatus of claim 36, wherein the profile generator defines a set
2 of drift-compensated target factors on a space of the drift-compensated principal
3 factors determined by a target-factor constructor operating on the drift-compensated
4 principal factors, applies the set of drift-compensated target factors to a profile
5 trajectory lying within a space of drift-compensated principal factors to obtain a
6 sequential set of target-factor weighting factors corresponding to the drift-
7 compensated target factors for the profile trajectory, and outputs to an output device
8 analytical results selected from the group consisting of a set of drift-compensated
9 scaled target-factor profiles derived from the set of target-factor weighting factors,
10 and the set of drift-compensated target factors.

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1 49. The apparatus of claim 48, wherein the target-factor constructor generates
2 a profile trajectory on a 3-dimensional projection of a 4-dimensional space of a set of
3 first-four, drift-compensated principal factors along with a reference tetrahedron the
4 vertices of which represent each of the first-four, drift-compensated principal factors;
5 encloses the profile trajectory within an enclosing tetrahedron with vertices centered on

6 end-points and in proximity to turning points of the profile trajectory, and with faces lying
7 essentially tangent to portions of the profile trajectory; and calculates the drift-
8 compensated target factors from the normed coordinates of the vertices of the enclosing
9 tetrahedron in terms of the drift-compensated principal factors.

1 50. The apparatus of claim 49, wherein the target-factor constructor in
2 generating the profile trajectory further calculates 4-space coordinates of a profile
3 trajectory of drift-compensated target-factor profiles on a 4-dimensional space to
4 produce four coordinates for each point in the profile trajectory, one coordinate for
5 each of the first-four, drift-compensated principal factors; reduces the dimensionality
6 of the coordinates of the profile trajectory by dividing each coordinate by a sum of all
7 four 4-space coordinates to produce normed coordinates for the profile trajectory;
8 and, plots the normed coordinates for the profile trajectory in a 3-dimensional space
9 the coordinate axes of which are edges of a reference tetrahedron the vertices of
10 which correspond to unit values for each of the first-four, drift-compensated principal
11 factors in a manner analogous to plotting of coordinates on a quaternary phase
12 diagram.

13

1 51. The apparatus of claim 48, wherein the profile generator further defines a
2 set of drift-compensated scaled target-factor profile values as the set of scaled target-
3 factor weighting factors, divides each drift-compensated scaled target-factor profile
4 value by a profile sensitivity factor for each constituent corresponding to the target factor
5 to provide a sensitivity-scaled target-factor profile value, divides each sensitivity-scaled
6 target-factor profile value for a given cycle number by the sum of all the sensitivity-

7 scaled target-factor profile values for the given cycle number to provide drift-
8 compensated compositional profile values at the given cycle number, and outputs the
9 drift-compensated compositional profile values as a set of drift-compensated
10 compositional profiles.

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1 52. An apparatus for compensating a plurality of sequential waveforms and
2 profiles derived therefrom for effects of drift, comprising a waveform analysis
3 system, wherein the waveform analysis system comprises:
4 a waveform-source device; and
5 a computer system, coupled to the waveform-source device, for analyzing
6 waveforms input from the waveform-source device, the computer system further
7 comprising a waveform processor for compensating a plurality of sequential
8 waveforms and profiles derived therefrom for effects of drift.

1 53. The apparatus of claim 52, wherein the waveform processor further
2 comprises:
3 a waveform transformer operating on a plurality of sequential waveforms
4 obtained from a waveform-source device to provide an array of drift-compensated
5 row vectors, wherein the array of drift-compensated row vectors constitutes a drift-
6 compensated array;
7 a principal-factor determinator operating on the drift-compensated array to
8 provide a set of drift-compensated principal factors; and
9 a profile generator operating on a profile trajectory of the drift-compensated
10 row vectors lying within a space of drift-compensated principal factors to provide a
11 set of drift-compensated scaled target-factor profiles.

1 54. The apparatus of claim 53, wherein the waveform transformer accepts
2 as input the plurality of sequential waveforms obtained from a waveform-source
3 device into the computer system, orders the waveforms in a primal array, wherein
4 each sequential waveform constitutes a successive row vector of the primal array,
5 and removes phase factors due to drift using a dephasor that transforms the primal
6 array into a drift-compensated array.

1 55. The apparatus of claim 54, wherein the dephasor that transforms the
2 primal array into the drift-compensated array applies a Fourier transform to the
3 primal array of row vectors to form an array of Fourier-transformed row vectors,
4 multiplies each Fourier-transformed row vector by a complex conjugate of each
5 Fourier-transformed row vector to form a squared moduli vector thereby removing
6 phase factors due to drift, takes the square root of each element of the squared
7 moduli vector to create a corresponding moduli vector, and forms a drift-
8 compensated array of moduli vectors by successively sequencing the moduli vectors
9 as successive drift-compensated row vectors in a drift-compensated array, wherein
10 the moduli vectors constitute moduli of Fourier-transformed waveforms.

1 56. The apparatus of claim 55 wherein the waveform transformer outputs
2 the drift-compensated row vectors of the drift-compensated array as a sequential
3 series of moduli of Fourier-transformed waveforms.

1 57. The apparatus of claim 54, wherein the dephasor that transforms the
2 primal array into the drift-compensated array fits each waveform in the primal array
3 using selected reference waveforms, calculates a corresponding reference weighting
4 factor for each reference waveform corresponding to each waveform in the primal
5 array, synthesizes a corresponding drift-compensated waveform given by the sum of
6 each selected reference waveform multiplied by the corresponding reference
7 weighting factor thereby removing phase factors due to drift, and forms a drift-
8 compensated array by successively sequencing the drift-compensated waveforms
9 as successive drift-compensated row vectors in the drift-compensated array.

1 58. The apparatus of claim 57 wherein the waveform transformer outputs
2 to an output device analytical results selected from the group consisting of the
3 selected reference waveforms used in the fitting procedure, the drift-compensated
4 row vectors of the drift-compensated array as a sequential series of drift-
5 compensated waveforms, reference weighting factors for each reference waveform
6 corresponding to each waveform in the primal array as a set of drift-compensated
7 reference-waveform profiles, and phase factors due to drift for each reference
8 waveform corresponding to each waveform in the primal array as a set of phase-
9 factor profiles.

1 59. The apparatus of claim 53 wherein the principal-factor determinator
2 comprises a factor analyzer.

1 60. The apparatus of claim 59, wherein the factor analyzer forms a
2 covariance array from the drift-compensated array, applies an eigenanalysis to the
3 covariance array to define a complete set of eigenvectors and eigenvalues, and
4 defines a set of drift-compensated principal factors as a subset of eigenvectors
5 determined by a selector operating on the complete set of eigenvectors.

1 61. The apparatus of claim 60, wherein the selector operates on the
2 complete set of eigenvectors to define the set of drift-compensated principal factors
3 as a first few eigenvectors corresponding to eigenvalues above a certain limiting
4 value.

1 62. The apparatus of claim 53 wherein the principal-factor determinator
2 comprises a linear-least-squares analyzer.

1 63. The apparatus of claim 62, wherein the linear-least-squares analyzer
2 selects a set of initial factors from the set of drift-compensated row vectors of the
3 drift-compensated array, performs a linear-least-squares decomposition with the set
4 of initial factors on the drift-compensated row vectors in the drift-compensated array
5 to provide a set of residue factors, and performs a Gram-Schmidt orthonormalization
6 on the combined set of initial factors and residue factors to provide drift-
7 compensated principal factors.

1 64. The apparatus of claim 53, wherein the profile generator defines a set
2 of drift-compensated target factors on a space of the drift-compensated principal
3 factors determined by a target-factor constructor operating on the drift-compensated

4 principal factors, applies the set of drift-compensated target factors to a profile
5 trajectory lying within a space of drift-compensated principal factors to obtain a
6 sequential set of target-factor weighting factors corresponding to the drift-
7 compensated target factors for the profile trajectory, and outputs to an output device
8 analytical results selected from the group consisting of a set of drift-compensated
9 scaled target-factor profiles derived from the set of target-factor weighting factors,
10 and the set of drift-compensated target factors.

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1 65. The apparatus of claim 64, wherein the target-factor constructor generates
2 a profile trajectory on a 3-dimensional projection of a 4-dimensional space of a set of
3 first-four, drift-compensated principal factors along with a reference tetrahedron the
4 vertices of which represent each of the first-four, drift-compensated principal factors;
5 encloses the profile trajectory within an enclosing tetrahedron with vertices centered on
6 end-points and in proximity to turning points of the profile trajectory, and with faces lying
7 essentially tangent to portions of the profile trajectory; and calculates the drift-
8 compensated target factors from the normed coordinates of the vertices of the enclosing
9 tetrahedron in terms of the drift-compensated principal factors.

1 66. The apparatus of claim 65, wherein the target-factor constructor in
2 generating the profile trajectory further calculates 4-space coordinates of a profile
3 trajectory of drift-compensated target-factor profiles on a 4-dimensional space to
4 produce four coordinates for each point in the profile trajectory, one coordinate for each
5 of the first-four, drift-compensated principal factors; reduces the dimensionality of the
6 coordinates of the profile trajectory by dividing each coordinate by a sum of all four 4-

- 7 space coordinates to produce normed coordinates for the profile trajectory; and, plots
- 8 the normed coordinates for the profile trajectory in a 3-dimensional space the coordinate
- 9 axes of which are edges of a reference tetrahedron the vertices of which correspond to
- 10 unit values for each of the first-four, drift-compensated principal factors in a manner
- 11 analogous to plotting of coordinates on a quaternary phase diagram.

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1 67. An article of manufacture comprising a program storage medium readable
2 by a computer, the medium tangibly embodying one or more programs of instructions
3 executable by the computer to perform a method for compensating a plurality of
4 sequential spectra and profiles derived therefrom for effects of drift, the method
5 comprising:

6 transforming a plurality of sequential spectra obtained from a spectrometer to
7 provide an array of drift-compensated row vectors, wherein the array of drift-
8 compensated row vectors constitutes a drift-compensated array;

9 performing a principal-factor determination on the drift-compensated array to
10 provide a set of drift-compensated principal factors; and,

11 generating drift-compensated scaled target-factor profiles from a profile trajectory
12 of the drift-compensated row vectors lying within a space of drift-compensated principal
13 factors.

14 68. The article of manufacture comprising a program storage medium
15 readable by a computer, the medium tangibly embodying one or more programs of
16 instructions executable by the computer to perform a method for compensating a
17 plurality of sequential spectra and profiles derived therefrom for effects of drift, the
18 method of claim 67 further comprising generating drift-compensated compositional
19 profiles from the set of drift-compensated scaled target-factor profiles.

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1 69. An article of manufacture comprising a program storage medium readable
2 by a computer, the medium tangibly embodying one or more programs of instructions
3 executable by the computer to perform a method for compensating a plurality of
4 sequential waveforms and profiles derived therefrom for effects of drift, the method
5 comprising:

6 transforming a plurality of sequential waveforms obtained from a waveform-
7 source device to provide an array of drift-compensated row vectors, wherein the array of
8 drift-compensated row vectors constitutes a drift-compensated array;

9 performing a principal-factor determination on the drift-compensated array to
10 provide a set of drift-compensated principal factors; and,

11 generating drift-compensated scaled target-factor profiles from a profile trajectory
12 of the drift-compensated row vectors lying within a space of drift-compensated principal
13 factors.